Spartan/Augustus Overview: Simplified Spherical Harmonics and Diffusion for Unstructured Hexahedral Lagrangian Meshes

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Available on-line at
`http://www.lanl.gov/Spartan/`

Outline

- Code Package Description

- Method Overview, Mesh Description

- SP_N

  - Equation Set

  - Properties

  - Solution Strategy

- Diffusion (P_1)

  - Equation Set

  - Properties

  - Solution Strategy

- Diffusion Results

- Future Work

Spartan/Augustus Code Package Description

Spartan: SP_N, 2 T + Multi-Group, Even-Parity Photon Transport Package with v/c corrections

Augustus: P_1 (Diffusion) Package

JTpack: Krylov Subspace Iterative Solver Package (by John Turner, ex-LANL)

UMFPACK: Unstructured Multifrontal Solver Package (an Incomplete Direct Method by Tim Davis, U of FL)

LINPACK: Direct Dense Linear Equation Solver Package

BLAS: Basic Linear Algebra Subprograms

Spartan/Augustus Code Size

Included files counted only once:

Spartan:	10213 lines, 57% comments
Augustus:	12872 lines, 60% comments
JTpack:	14167 lines, 54% comments
UMFPACK:	15393 lines, 58% comments
BLAS:	7467 lines, 48% comments
LINPACK:	6926 lines, 52% comments
Total	67038 lines, 56% comments

With includes:

Spartan:	14080 lines, 71% comments
Augustus:	31595 lines, 78% comments
JTpack:	36009 lines, 73% comments
UMFPACK:	15393 lines, 58% comments
BLAS:	7467 lines, 48% comments
LINPACK:	6926 lines, 52% comments
Total	111470 lines, 73% comments

- Energy/Temperature Discretization

  - Solves 2 T + Multi-Group Even-Parity Equations
  - Can yoke T_e and T_i together to make 1 T
  - Can use a single-group radiation treatment to make 3 T

- Angular Discretization

  - Uses Simplified Spherical Harmonics — SP_N
  - Can do a P_1 (diffusion-like) solution

- Spatial Discretization

  - SP_N decouples equations into many diffusion equations
  - Diffusion equations are solved by Augustus

- Temporal Discretization

  - Linearized implicit discretization
  - Equivalent to one pass of a Newton solve
  - Iteration strategy:

    * Source iteration
    * DSA acceleration
    * LMFG acceleration

Method Overview: Augustus

- Spatial Discretization

  – Morel-Hall asymmetric diffusion discretization

  – Support Operator symmetric diffusion discretization

  – Hall symmetric diffusion discretization (2-D, x-y only)

- Temporal Discretization

  – Backwards Euler implicit discretization

- Matrix Solution

  – Krylov Subspace Iterative Methods

    * JTpack: GMRES, BCGS, TFQMR
    * Preconditioners:
      · JTpack: Jacobi, SSOR, ILU
      · Low-order version of Morel-Hall discretization that is a smaller, symmetric system and is solved by CG with SSOR (from JTpack)

  – Incomplete Direct Method - UMFPACK

Mesh Description

Multi-Dimensional Mesh:

Dimension	Geometries	Type of Elements
1-D	spherical, cylindrical or cartesian	line segments
2-D	cylindrical or cartesian	quadrilaterals or triangles
3-D	cartesian	hexahedra or degenerate hexahedra (tetrahedra, prisms, pyramids)

all with an unstructured (arbitrarily connected) format.
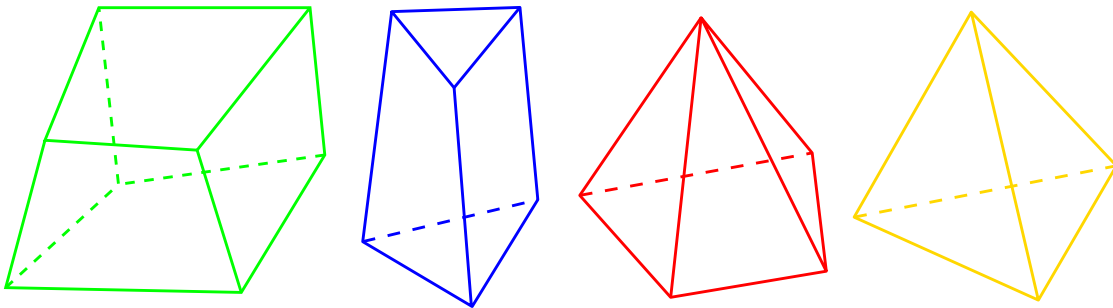
This presentation will assume a 3-D mesh.

Simplified Spherical Harmonics (SP_N) Even-Parity Equation Set

Radiation transport equations:

$$\frac{1}{c}\frac{\partial}{\partial t}\xi_{m,g} + \overrightarrow{\nabla} \cdot \overrightarrow{\Gamma}_{m,g} + \sigma_g^t \xi_{m,g} = \sigma_g^s \phi_g + \sigma_g^e B_g + \mathcal{C}_g^s \, ,$$

$$\frac{1}{c}\frac{\partial}{\partial t}\overrightarrow{\Gamma}_{m,g} + \mu_m^2 \overrightarrow{\nabla}\xi_{m,g} + \sigma_g^t \overrightarrow{\Gamma}_{m,g} = \overrightarrow{\mathcal{C}}^v_{m,g}$$

for $m = 1, M$, and $g = 1, G$.

Temperature equations:

$$C_{vi}\frac{\partial T_i}{\partial t} = \alpha\left(T_e - T_i\right) + Q_i \, ,$$

$$C_{ve}\frac{\partial T_e}{\partial t} = \alpha\left(T_i - T_e\right) + Q_e + \sum_{g=1}^{G}\left(\sigma_g^a \phi_g^{(0)} - \sigma_g^e B_g\right) \, ,$$

where

$$\xi_{m,g} = \text{Even-parity pseudo-angular energy intensity,}$$

$$\overrightarrow{\Gamma}_{m,g} = \text{Even-parity pseudo-angular energy current,}$$

$$
\mathcal{C}_g^s = \left(\sigma_g^a - \sigma_g^s\right) \overrightarrow{F}_g^{(0)} \cdot \frac{\overrightarrow{v}}{c} \, ,
$$

$$
\overrightarrow{\mathcal{C}}_{m,g}^v = 3\mu_m^2 \sigma_g^t \left(P_g + \phi_g\right) \frac{\overrightarrow{v}}{c} \, ,
$$

$$
\phi_g = \sum_{m=1}^{M} \xi_{m,g}\, w_m \, ,
$$

$$
P_g = \sum_{m=1}^{M} \xi_{m,g}\, \mu_m^2\, w_m \, ,
$$

$$
\overrightarrow{F}_g = \sum_{m=1}^{M} \overrightarrow{\Gamma}_{m,g}\, w_m \, ,
$$

$$
\phi_g^{(0)} = \phi_g - 2\, \overrightarrow{F}_g^{(0)} \cdot \frac{\overrightarrow{v}}{c} \, ,
$$

$$
\overrightarrow{F}_g^{(0)} = \overrightarrow{F}_g - \left(P_g + \phi_g\right) \frac{\overrightarrow{v}}{c} \, ,
$$

$$
M = \left(N + 1\right)/2 \, .
$$

Simplified Spherical Harmonics (SP_N) Properties

- SP_1 and P_1 equations are identical.

- SP_N and P_N equations are identical in 1-D slab geometry.

- Rotationally invariant $\longrightarrow$ no ray effects.

- SP_N is a non-convergent method. It is an asymptotic approximation associated with the diffusion limit. As $N \longrightarrow \infty$, the solution doesn't necessarily converge to the true answer.

- SP_N has almost the same accuracy for lower orders as S_N if the solution is approximately locally 1-D, but is much cheaper.

Simplified Spherical Harmonics (SP_N) Properties (cont)

- With DSA and LMFG acceleration, SP_N costs $MG + G + 1$ diffusion solutions for every outer iteration.

- Unlike the diffusion equation, the SP_N equations propagate information at a finite speed. For radiation, this speed approaches c from below as the order of approximation is increased.

- Order N unknowns for SP_N, vs. order N^2 unknowns for P_N and S_N.

- In a homogeneous region, SP_N and P_N scalar flux solutions satisfy same equation, except with different boundary conditions.

Simplified Spherical Harmonics (SP_N) Temporal Discretization

Radiation transport equations:

$$\frac{1}{c}\frac{\partial}{\partial t}\xi_{m,g} + \overrightarrow{\nabla}\cdot\overrightarrow{\Gamma}_{m,g} + \sigma_g^t\xi_{m,g} = \sigma_g^s\phi_g + \sigma_g^e B_g + \mathcal{C}_g^s \, ,$$

$$\frac{1}{c}\frac{\partial}{\partial t}\overrightarrow{\Gamma}_{m,g} + \mu_m^2\overrightarrow{\nabla}\xi_{m,g} + \sigma_g^t\overrightarrow{\Gamma}_{m,g} = \overrightarrow{\mathcal{C}}{}_{m,g}^v$$

for $m = 1, M$, and $g = 1, G$.

Temperature equations:

$$C_{vi}\frac{\partial T_i}{\partial t} = \alpha\left(T_e - T_i\right) + Q_i \, ,$$

$$C_{ve}\frac{\partial T_e}{\partial t} = \alpha\left(T_i - T_e\right) + Q_e + \sum_{g=1}^{G}\left(\sigma_g^a\phi_g^{(0)} - \sigma_g^e B_g\right) \, ,$$

where

$$
\begin{aligned}
Blue &= \text{Implicit or backwards Euler terms,}\\
Magenta &= \text{Explicit or extrapolated implicit terms,}\\
Red &= \text{Implicit terms accelerated by DSA,}\\
Green &= \text{Linearized implicit terms accelerated by LMFG.}
\end{aligned}
$$

This is not quite accurate — it's actually more complicated than this — but this captures the flavor of the temporal discretization.

Simplified Spherical Harmonics (SP_N) Source Iteration Strategy

- SP_N Equations: Red and Green terms are treated explicitly, equations decouple into $M \times G$ separate diffusion equations

- DSA Equations: summing over angle and treating Red terms implicitly leads to G separate diffusion equations, which provide an angle-constant update

- LMFG Equation: summing over group and treating Green terms implicitly leads to a single diffusion equation, which provides a spectrum-scaled update

- These equations are solved repeatedly until the Red and Green terms converge

$$\alpha \frac{\partial \Phi}{\partial t} - \overrightarrow{\nabla} \cdot D \overrightarrow{\nabla} \Phi + \overrightarrow{\nabla} \cdot \overrightarrow{J} + \sigma \Phi = S$$

Which can be written

$$\alpha \frac{\partial \Phi}{\partial t} + \overrightarrow{\nabla} \cdot \overrightarrow{F} + \sigma \Phi = S$$
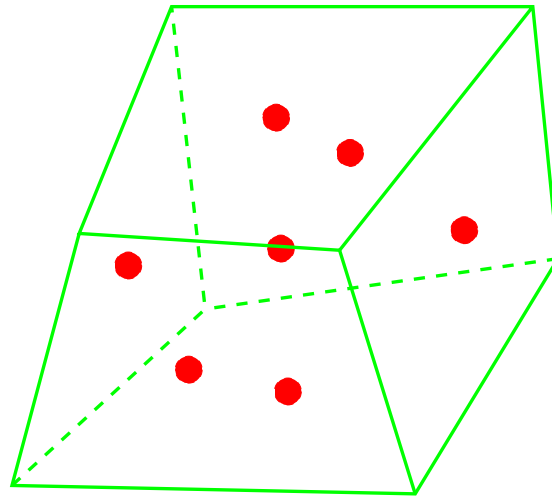
$$\overrightarrow{F} = -D \overrightarrow{\nabla} \Phi + \overrightarrow{J}$$

Where

$$
\begin{array}{rcl}
\Phi & = & \text{Intensity} \\
\overrightarrow{F} & = & \text{Flux} \\
D & = & \text{Diffusion Coefficient} \\
\alpha & = & \text{Time Derivative Coefficient} \\
\sigma & = & \text{Removal Coefficient} \\
S & = & \text{Intensity Source Term} \\
\overrightarrow{J} & = & \text{Flux Source Term}
\end{array}
$$

Diffusion Discretization Method Properties

All three methods:

- Are cell-centered – balance equations are done over a cell

- Require cell-centered and face-centered unknowns to rigorously treat material discontinuities

- Preserve the homogeneous linear solution, and are second-order accurate

- Reduce to the standard cell-centered operator for an orthogonal mesh

- Maintain local energy conservation

Diffusion Discretization Method Properties (cont)

- Morel-Hall Asymmetric Method

  - Described in

    Michael L. Hall, and Jim E. Morel. A Second-Order Cell-Centered Diffusion Differencing Scheme for Unstructured Hexahedral Lagrangian Meshes. In *Proceedings of the 1996 Nuclear Explosives Code Developers Conference (NECDC), UCRL-MI-124790*, pages 359–375, San Diego, CA, October 21–25 1996. LA-UR-97-8.

    which is an extension of

    J. E. Morel, J. E. Dendy, Jr., Michael L. Hall, and Stephen W. White. A Cell-Centered Lagrangian-Mesh Diffusion Differencing Scheme. Journal of Computational Physics, 103(2):286-299, December 1992.

    to 3-D unstructured meshes, with an alternate derivation.

- Hall Symmetric Method:

  - Based on the above method, but only applicable in 2-D x-y.

- Support Operator Symmetric Method:

  - Extension of the method described in

    Mikhail Shashkov and Stanly Steinberg. Solving Diffusion Equations with Rough Coefficients in Rough Grids. Journal of Computational Physics, 129:383-405, 1996.

    to 3-D unstructured meshes, with an alternate derivation.

Diffusion Discretization Stencil

The flux at a given face, for example the $+k$-face,

$$\overrightarrow{F}^{n+1}_{+k} = -D_{c,+k}\overrightarrow{\nabla}\Phi^{n+1} + \overrightarrow{J_{+k}}$$

is defined using this stencil:
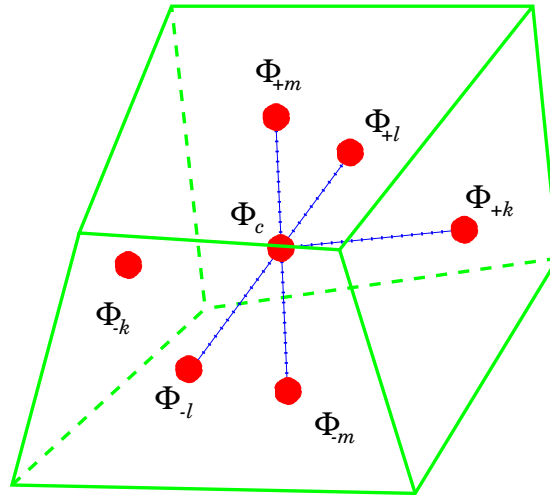
in the Asymmetric Method. The Support Operator Method uses all seven unknowns within a cell to define the face flux.

Each cell has a cell-centered conservation equation which involves all six face fluxes, and gives a stencil which includes all seven unknowns within the cell (in both methods).
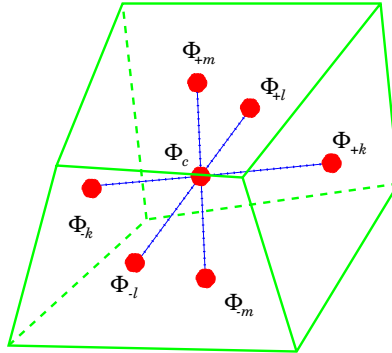
To close the system, an equation relating the fluxes on each side of a face is added for every face in the problem. This gives the following stencil:
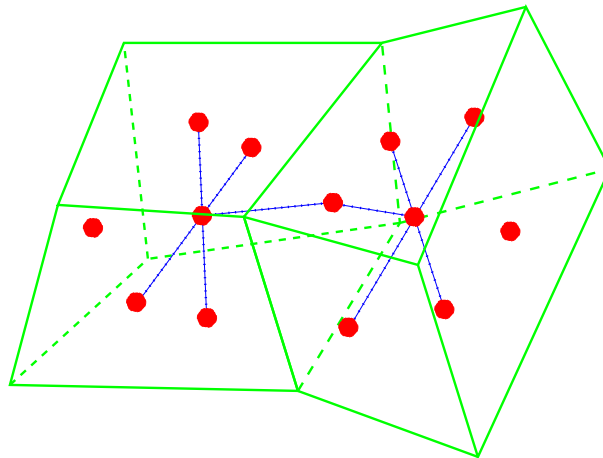
in the Asymmetric Method. The Support Operator Method uses all thirteen unknowns within a cell-cell pair to define the face equation.

Algebraic Solution

- Main Matrix System (Asymmetric Method):

  - Asymmetric – must use an asymmetric solver like GMRES, BCGS or TFQMR

  - Size is $(4n_c + n_b/2)$ squared

  - Maximum of 11 non-zero elements per row

- Main Matrix System (Support Operator Method):

  - Symmetric – can use CG to solve

  - Size is $(4n_c + n_b/2)$ squared

  - Maximum of 13 non-zero elements per row

- Preconditioner for Krylov Space methods is a Low-Order Matrix System:

  - Assume orthogonal: drop out minor directions in flux terms

  - Symmetric – can use standard CG solver

  - Size is n_c squared

  - Maximum of 7 non-zero elements per row

# Results: Sample Augustus Problem

- 3-D Kershaw-Squared Mesh

- Constant properties

- No removal or sources

- Reflective boundaries on 4 sides

- Source and vacuum boundary conditions on opposite sides

- Analytic solution - linear

- Grid size - $20 \times 20 \times 20 = 8000$ nodes, 6859 cells

- 50 time steps, 15 s / time step on IBM RS/6000 Scalable POWERparallel System, SP2
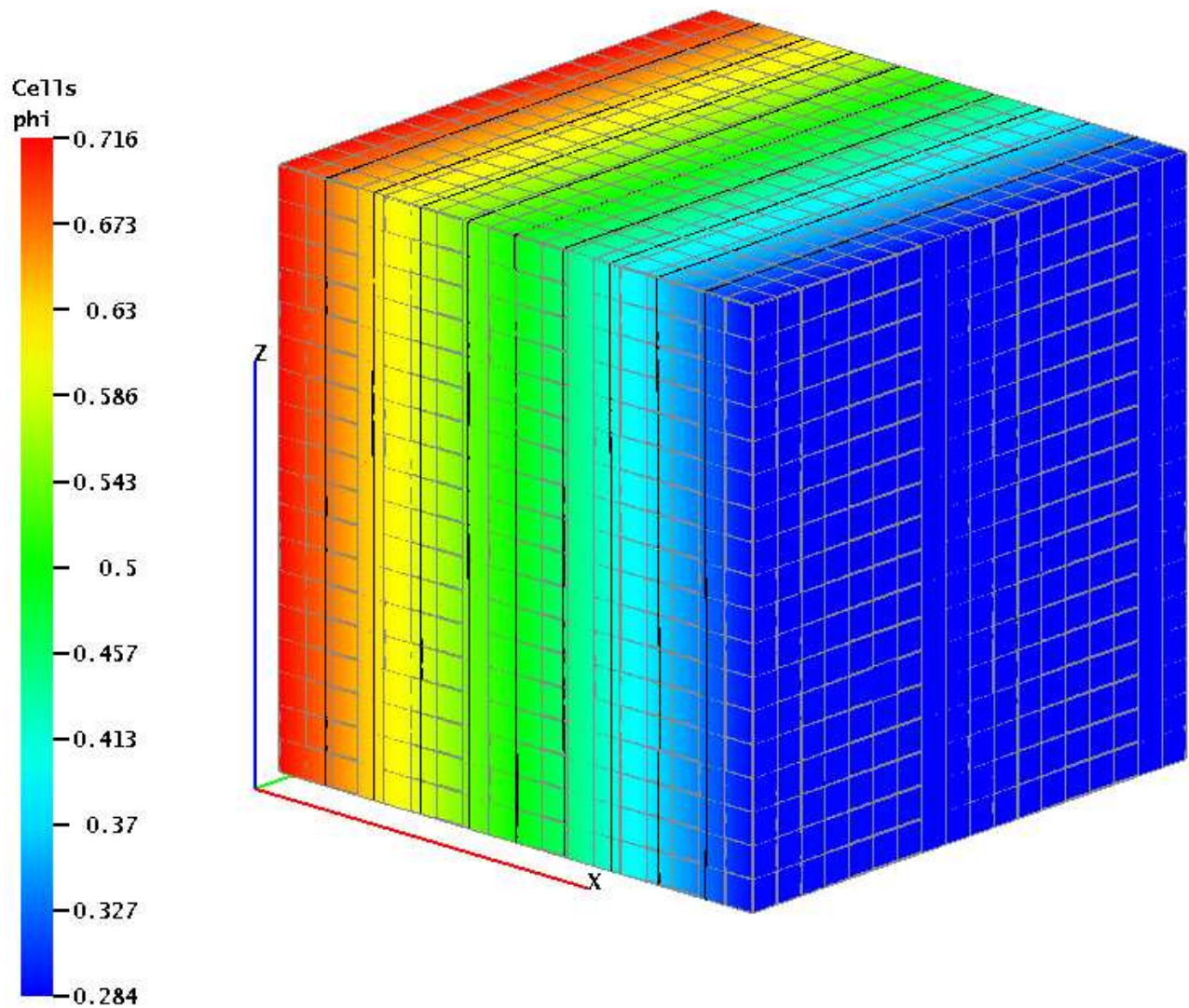
Results: Sample Problem
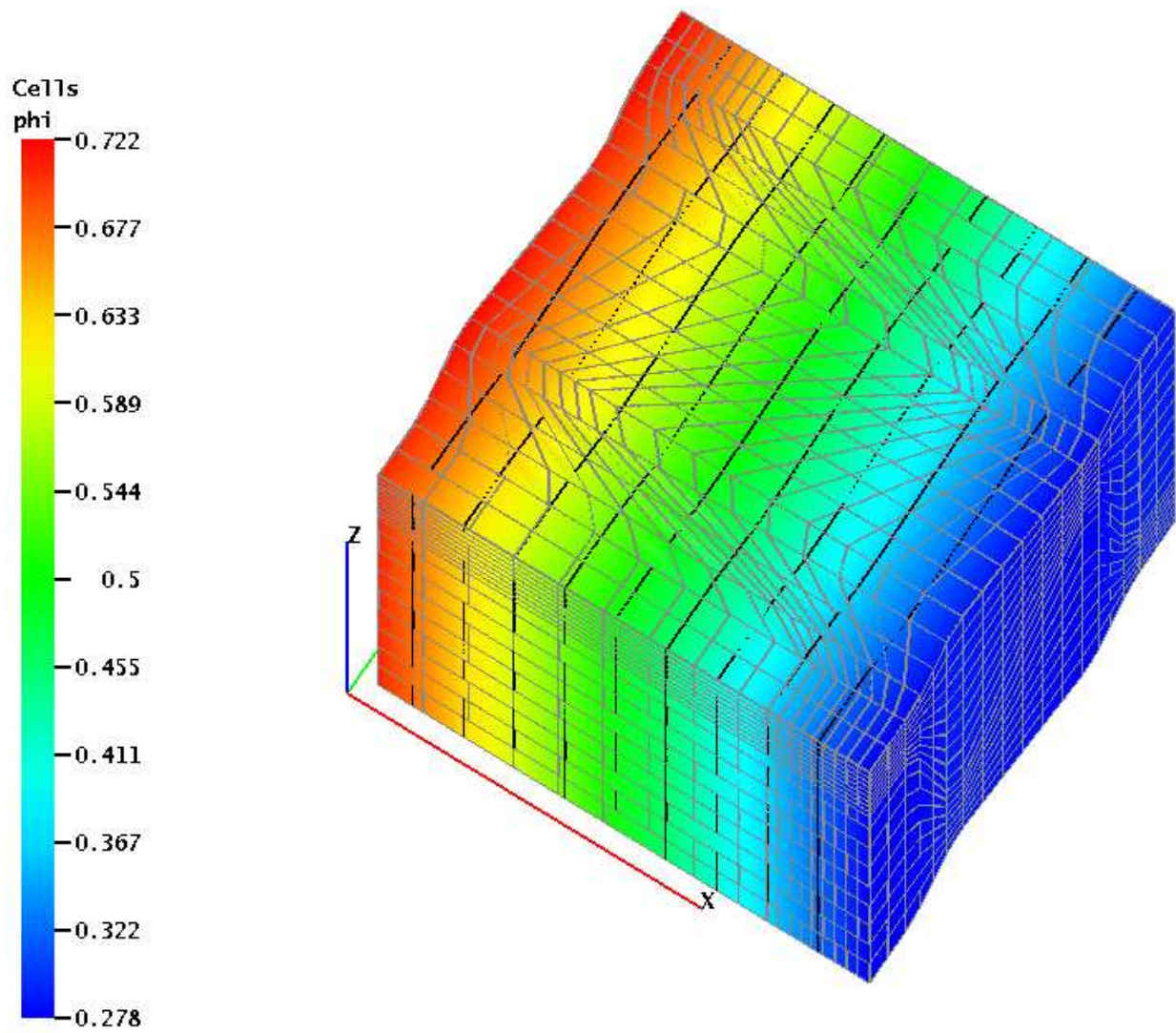
Actual Mesh (Cell Nodes)
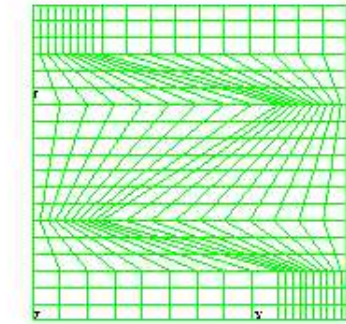
Dual Mesh (Cell Centers)
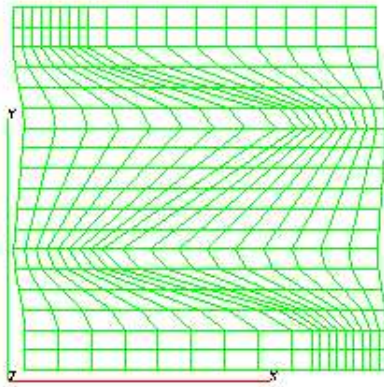
Results: Sample Problem

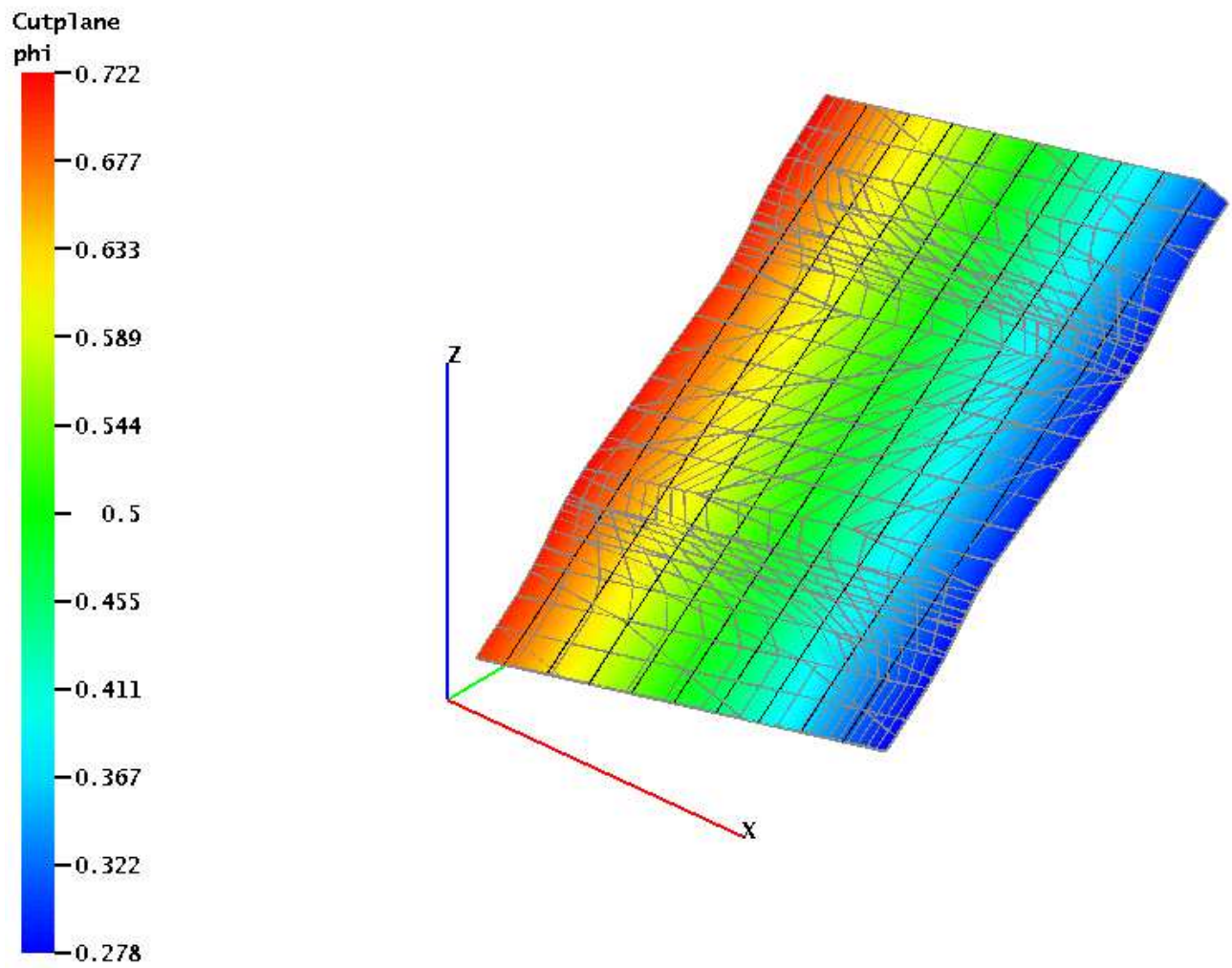Orthogonal Mesh Steady State Solution

Results: Sample Problem

Kershaw-Squared Mesh Steady State

Results: Sample Problem

Kershaw–Squared Random Cutplane

Future Work

- Parallel (JTpack90, PGSlib, SPAM)

- Object-based, design-by-contract F90

- Generic programming?

- Integrated documentation (HTML, PS)

- Newton-Krylov solution method?

- Alternate angular discretization?

- Self-adjoint equation set?